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Fast Refrigerant Property Calculations Using Interpolation-Based Methods

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ABSTRACT

An interpolation-based method for computing refrigerant properties which can be used in simulations of vapor-compression air-conditioning equipment is presented. This method uses bicubic functions to interpolate between samples of the Helmholtz energy surface as a function of temperature and density. Three beneficial characteristics of this method are discussed: speed, accuracy, and consistency, as well as a means for using a variety of different independent variables are also presented. The implementation of this method is discussed, and experimental results for property calculations for refrigerant R-134a are presented which compare favorably to standard Newton-based equation of state methods.

1 INTRODUCTION

Simulation techniques have become an increasingly important tool for improving the performance of vapor compression air-conditioning equipment, due to the strongly coupled dynamics manifest in these systems and the fact that experimental platforms are quite expensive to construct and maintain. One critical aspect of any simulation of a vapor compression air-conditioning system is the representation of the refrigerant's thermodynamic properties. These properties constitute an important constraint on the system behavior, as the state of the refrigerant at any point in the refrigerant cycle is fixed by measuring the appropriate number of properties for the refrigerant state. Once the state is fixed, any other property of the fluid (e.g., density, specific enthalpy, or specific entropy) is theoretically uniquely determined, and can be computed with the appropriate equation of state (EOS).

Unfortunately, this theory does not describe how to proceed with these calculations. As these property calculations are essential to understanding the behavior of physical systems which incorporate thermofluids, a variety of methods for calculating fluid properties, which span a wide range of complexity, have been developed. While simple methods, such as the Van der Waals equation, represent the properties of some fluids remarkably well, more complex EOS formulations have been developed, such as today's multiparameter equations of state (Span, 2000), that are able to represent the thermophysical behavior of fluids extremely accurately to meet the demand for more precision. Refrigerants that are used in contemporary vapor compression equipment usually require these modern representations to accurately characterize their behavior.

Two popular methods for computing refrigerant properties in air-conditioning simulations include the software package Refprop and general precomputed lookup tables. Refprop (Lemmon *et al.*, 2010) is a program written by NIST in the United States which includes state-of-the-art EOS representations for a wide variety of fluids and can perform a wide range of thermofluid property calculations for both pure fluids and nearly arbitrary mixtures of fluids. However, Refprop is mainly designed for the exploration and calculation of the thermodynamic properties of fluids, rather than for the particular inclusion of refrigerant property calculations in simulations of vapor compression equipment. Alternatively, many air-conditioner simulations use precomputed lookup tables, where the desired properties (e.g., specific enthalpy) are computed from a set of measured variables (e.g., temperature and pressure) before running the simulation, and then the simulation simply looks up the corresponding property value at runtime.

While both of these property calculation methods can be effective in simulations of vapor compression equipment, each has significant shortcomings. Refprop is designed to allow the user a great deal of flexibility in the choice of

pure fluid or mixture to simulate, rather than the speed of simulation; when it is incorporated into a simulation which makes tens of thousands of property calls, its calculation time quickly limits the overall simulation speed. Precomputed lookup tables, on the other hand, have the advantage of being very fast, but basic lookup tables that do not perform any interpolation typically have an accuracy which is strongly dependent upon the sampling density of the property.

New applications of simulation, such as simulations of hybrid vehicle air-conditioning systems over many drive profiles and long periods of time, suggest a need for property calculation methods which are both fast and accurate. Moreover, the consistency of these property calculations is also essential for simulations of air-conditioning equipment. For example, the specific enthalpy \hat{h} of a fluid can be computed as a function of measurements of temperature T and pressure p , where the hat denotes the fact that this property is computed rather than measured. This new value of \hat{h} can then be used with p to calculate \hat{T} . Ideally, the resulting value of \hat{T} will be identical to the original measurement T , but in general the difference between these two values will produce a nonzero residual r . Because a variety of different measurements are used in these simulations for many different computations, these calculations must be consistent; that is, it is important that the property calculation method be designed to minimize the size of r .

Previous work has been done to develop new fast and accurate property computation methods for the simulation of air-conditioning equipment. Ding *et al.* (2005, 2007, 2009) developed a polynomial interpolation method for fluids over a specified range of operating conditions. Consistency conditions are also enforced through the particular construction of the regression method that is used to calculate the coefficients of the interpolating polynomials from the property data obtained from Refprop. The authors report significant reduction in the computation time for properties for R22 and R407C, as well as errors that are at or below 1.5%. An alternative method was developed by Kunick *et al.* (2008, 2009) that uses a biquadratic spline interpolation method to compute the properties of water and CO₂. These splines are fit from specific combinations of data, e.g., $T(p, h)$, $s(p, h)$, over a grid of measurements which is specified ahead of time. This spline representation is desirable because it represents the desired property as a continuous surface, rather than just samples of a surface. Some consistency relations can also be enforced for this method because the inverse calculations can be computed algebraically. Reported results demonstrate a significant reduction in the computational time as well as an average deviation of less than 10^{-7} .

The method described in this paper also uses an interpolation method to represent the properties on the surface, but the main distinction of this paper is that particular state function is chosen to interpolate because it has particularly useful characteristics. As the Helmholtz energy is a fundamental equation of state, the creation of a single set of interpolating functions for the Helmholtz energy can be used to calculate all of the fluid's properties. The use of the interpolating functions ensures both high accuracy and high speed, and the use of the Helmholtz energy implicitly ensures the consistency of all of the calculated state functions, rather than relying upon the accuracy of the regression that is used to generate the coefficients of the interpolating functions.

The remainder of this paper describes the property calculation method that was developed in response to the need for a method which addresses the three requirements of speed, accuracy, and consistency. Section 2 describes the rationale for the underlying structure of the method, while Section 3 discusses specific details pertaining to the implementation of the method. Section 4 provides an application of this method to calculations for R-134a of the superheated vapor region up to and including the saturation line, and results demonstrating this method's efficacy are then presented. Conclusions and potential directions for future work are outlined in Section 5.

2 STRUCTURE OF METHOD

As can be seen from (Ding *et al.*, 2005, 2007, 2009, Kunick *et al.*, 2009, Zhao *et al.*, 2009), interpolating functions are attractive for the purpose of characterizing a set of desired properties as a function of a different set of measured properties. These methods effectively parameterize a property of the fluid over a region defined in terms of the independent variables; for example, h can be parameterized as $h(T, p)$. These methods generally cannot be easily used to calculate the range of other properties, however. The method described in Kunick is quite interesting because it facilitates both the direct and inverse computation by virtue of its structure, thereby enforcing consistency upon the variables that were fit.

When endeavoring to ensure consistency as well as speed and accuracy, it can be advantageous to interpolate a function which can be easily manipulated into a wide variety of forms. Current methods for characterizing the thermodynamic properties of fluids fit functional forms to a fundamental equation of state, rather than a volumetric equation of state, because fundamental equations of state allow all other state functions to be easily calculated by differentiation (Sandler, 2006). For example, Refprop characterizes many of its fluids in terms of the Helmholtz energy $A(T, \rho)$, which is a fundamental EOS. A few of the properties that can be calculated from the Helmholtz energy (Lemmon *et al.*, 2009, Span, 2000) are as follows:

$$p = \rho^2 \left(\frac{\partial a}{\partial \rho} \right)_T \quad (1)$$

$$\frac{s}{R} = -\frac{1}{R} \left(\frac{\partial a}{\partial T} \right)_\rho \quad (2)$$

$$\frac{u}{RT} = \frac{a + TS}{RT} \quad (3)$$

$$\frac{h}{RT} = \frac{u + p/\rho}{RT} \quad (4)$$

$$\frac{c_v}{RT} = \frac{1}{R} \left(\frac{\partial u}{\partial T} \right)_\rho \quad (5)$$

where a denotes the specific Helmholtz energy. Other properties and derivatives of properties can be computed analogously.

While the structure of these equations makes it clear how to compute properties given T and ρ as independent variables, additional work is required to compute all possible state functions from other independent variables, such as p and h . In general, the approach that is used is that an initial guess for (T, ρ) is posited and used to calculate A , from which the related values of the independent variables \hat{p} and \hat{h} are calculated. The residuals $(p - \hat{p})$ and $(h - \hat{h})$ are then used to iteratively improve the initial guesses for (T, ρ) until the magnitudes of the residuals are reduced below a set tolerance. When this threshold is reached, the values of A, T, ρ are presumed to be close enough to the true value that all desired state functions can be computed from these values.

The main appeal of this method is that it ensures both consistency and accuracy. By properly constructing iterative root-finding algorithms that facilitate the computation of A from any initial set of two independent variables, this approach can calculate any dependent state function from the same value of A . Since the same value of A is used to calculate all properties, these properties are guaranteed to be consistent. The accuracy of the calculated values (within the constraints of the mathematical assumptions required by the solution algorithm) can also be controlled through the choices of tolerances.

The aspects of the a fundamental EOS that make it particularly useful for contemporary property calculations also recommend its use as the function to be interpolated when simulating vapor compression air-conditioning equipment. More specifically, it is possible to consistently calculate any state function at any point in the interpolated region by using interpolation functions to model the Helmholtz energy surface $A(T, \rho)$. This removes the limitation inherent in other approaches, where the calculations are only consistent among the state functions used to determine the coefficients of the interpolating functions.

The relationship between A and the other state functions also makes it possible to consistently calculate the properties from independent variables other than (T, ρ) . Since the interpolating functions contain polynomial terms that are functions of (T, ρ) , they can be easily manipulated to calculate the derivatives that are proportional to other terms, such as the pressure p . The relationship between (T, ρ) and (T, p) can then be inverted so that the value of the surface A can be determined as a function of the independent variables T and p . Once the particular value for A is known, the corresponding values of (T, ρ) can be quickly computed, and any other desired state function can be easily computed as well. There are a limited number of combinations of independent variables for which this approach is not effective, and for which Newton iterations must instead be used to locate the correct values of (T, ρ) to determine the desired properties.

This approach to property calculation might be described as using the Helmholtz energy as a type of “pivot” variable, where the two independent variables are first related to A , this value of A is related to the corresponding values of (T, ρ) , and then any desired property can be obtained. The three stated objectives of the property calculation method can thus be reached: consistency can be ensured by using A to generate all of the properties, speed can be obtained by using a suitable interpolation method, and accuracy can be obtained by choosing the appropriate sampling density of the $A(T, \rho)$ surface.

3 IMPLEMENTATION

This approach to the calculation of state functions was tested with an interpolation method which used bicubic functions to approximate $A(T, v)$ on a uniform mesh covering the region of interest in the T, v domain¹ (Spath, 1993, 1995). Due to the complexity of the mathematical notation required to implement this method, the description of this implementation is broken down into a series of subsections. First, the method by which the coefficients of the interpolating functions are determined on each grid cell is explained. Since the manner by which the pressure p and the specific entropy s are calculated from (T, v) is the most straightforward, it is discussed next. The method for calculating v from (T, p) and T from (s, v) is then discussed due to its slightly higher complexity, and then the method for calculating (T, v) from (s, p) is presented. Finally, implementation details pertaining to the identification of the correct grid cell are presented, since this information is crucial to the method’s proper function.

3.1 Determining the Coefficients of the Bicubic Functions

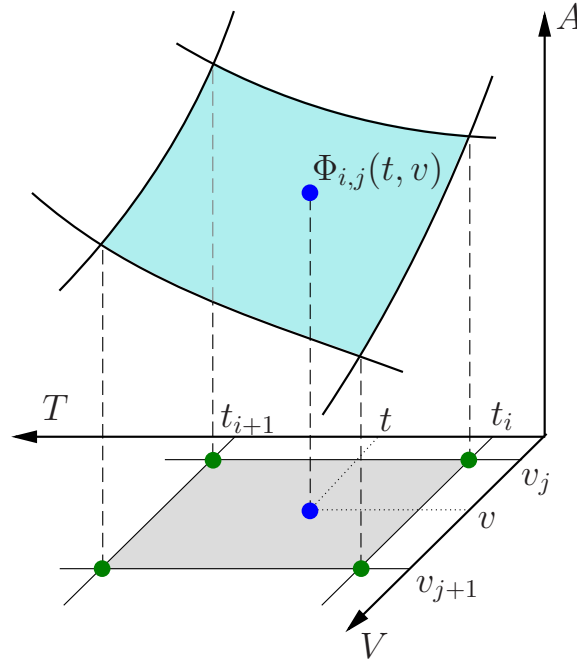


Figure 1: Helmholtz free energy on a grid cell.

In each grid cell, the value of A is approximated by a bicubic function $\Phi_{i,j}$, which is given by

$$\Phi_{i,j}(T, v) = \sum_{k=0}^3 \sum_{\ell=0}^3 a_{k\ell} (T - T_i)^k (v - v_j)^\ell \quad (6)$$

for $(T, v) \in (T_i, T_{i+1}) \times (v_j, v_{j+1})$. The 16 unknown coefficients $a_{k\ell}$ in Equation (6) can be computed from a set of 16 equations. The four equations for the point (i, j) are provided below; similar equations for adjacent vertices of the grid

¹Note that this method parameterized A in terms of the specific volume v , rather than the density ρ .

cell $(i + 1, j)$, $(i, j + 1)$, and $(i + 1, j + 1)$ are structured analogously.

$$\begin{aligned}\Phi_{i,j}(T_i, v_j) &= A(t_i, v_j), & \frac{\partial \Phi_{i,j}}{\partial T}(T_i, v_j) &= \frac{\partial A}{\partial T}(T_i, v_j), \\ \frac{\partial \Phi_{i,j}}{\partial v}(T_i, v_j) &= \frac{\partial A}{\partial v}(T_i, v_j), & \frac{\partial^2 \Phi_{i,j}}{\partial T \partial v}(T_i, v_j) &= \frac{\partial^2 A}{\partial T \partial v}(T_i, v_j).\end{aligned}$$

As the above functions are linear in $a_{k\ell}$, $k, \ell = 0, 1, 2, 3$, these coefficients can be easily calculated after the values of A and its derivatives at the four grid cell corner points are computed from the full multiparameter EOS.

For notational simplicity, (6) can also be rewritten in a matrix form as

$$\Phi_{i,j}(T, v) = \phi_{i,j}(\tau, v) = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \end{bmatrix} \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 1 \\ v \\ v^2 \\ v^3 \end{bmatrix} \quad (7)$$

where $\tau = T - T_i$, $v = v - v_j$.

3.2 Computing p and s from (T, v)

As stated previously, the relation between A and p is given by

$$p(T, v) = -\frac{\partial A}{\partial v}(T, v) \quad (8)$$

Given the bicubic approximation of A on a grid cell $(T, v) \in [T_i, T_{i+1}] \times [v_i, v_{i+1}]$, the pressure p can be computed by

$$\begin{aligned}p &= F_p(T, v) = -\frac{\partial \Phi_{i,j}}{\partial v}(T, v) = -\frac{\partial \phi_{i,j}}{\partial v}(\tau, v) = f_p(\tau, v) \\ &= -\begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \end{bmatrix} \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2v \\ 3v^2 \end{bmatrix} \\ &= -\begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \end{bmatrix} \begin{bmatrix} a_{01} & a_{02} & a_{03} \\ a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 1 \\ 2v \\ 3v^2 \end{bmatrix} \quad (9)\end{aligned}$$

Similarly, from the fact that

$$s(T, v) = -\frac{\partial A}{\partial T}(T, v),$$

the specific entropy can be approximated by

$$\begin{aligned}s &= F_s(T, v) = -\frac{\partial \phi_{i,j}}{\partial \tau}(\tau, v) \\ &= f_s(\tau, v) \\ &= -\begin{bmatrix} 1 & 2\tau & 3\tau^2 \end{bmatrix} \begin{bmatrix} a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 1 \\ v \\ v^2 \\ v^3 \end{bmatrix} \quad (10)\end{aligned}$$

3.3 Computing v from (p, t) and T from (s, v)

From (9), it is clear that for fixed T value, p is a quadratic function in v . Therefore, v can be easily determined by finding the root of the quadratic function. Specifically, let $c_{v2}(T) = 3a_{33}\tau^3 + 3a_{23}\tau^2 + 3a_{13}\tau + 3a_{03}$, $c_{v1}(T) = 2a_{32}\tau^3 + 2a_{22}\tau^2 + 2a_{12}\tau + 2a_{02}$, and $c_{v0}(T, p) = 2a_{31}\tau^3 + 2a_{21}\tau^2 + 2a_{11}\tau + 2a_{01} + p$, then p and v satisfy the following equation

$$c_{v2}(T)v^2 + c_{v1}(T)v + c_{v0}(T, p) = 0$$

Hence v is given by

$$v = F_v(T, p) = v_j + v = v_j + \frac{-c_{v1}(T) + \sqrt{c_{v1}^2(T) - 4c_{v2}(T)c_{v0}(T, p)}}{2c_{v2}(T)} \quad (11)$$

The other root is omitted because it is not feasible.

Similarly, for given s and v , let $c_{\tau2}(v) = 3a_{33}v^3 + 3a_{32}v^2 + 3a_{31}v + 3a_{30}$, $c_{\tau1}(v) = 2a_{23}v^3 + 2a_{22}v^2 + 2a_{21}v + 2a_{20}$, $c_{\tau0}(s, v) = a_{13}v^3 + a_{12}v^2 + a_{11}v + a_{10} + s$, then

$$T = F_t(s, v) = T_i + \tau = T_i + \frac{-c_{\tau1}(v) - \sqrt{c_{\tau1}^2(v) - 4c_{\tau2}(v)c_{\tau0}(s, v)}}{2c_{\tau2}(v)} \quad (12)$$

3.4 Computing (s, p) from (T, v)

Unlike the other types of calculations introduced previously, T or v cannot be calculated analytically when only the pair of state functions (s, p) is provided. In this case, it is more convenient to compute the corresponding T and v simultaneously using Newton's method. Specifically, τ and v are obtained by solving the following equation

$$f(\tau, v) = \begin{bmatrix} f_p(\tau, v) - p \\ f_s(\tau, v) - s \end{bmatrix} = 0 \quad (13)$$

Let τ_i and v_i be the estimated root values in the current step. The Newton's update for the next step is

$$\begin{aligned} \begin{bmatrix} \tau_{k+1} \\ v_{k+1} \end{bmatrix} &= \begin{bmatrix} \tau_k \\ v_k \end{bmatrix} - \nabla F^{-1}(\tau_k, v_k) F(\tau_k, v_k) \\ &= \begin{bmatrix} \tau_k \\ v_k \end{bmatrix} - \begin{bmatrix} \frac{\partial F_p}{\partial \tau}(\tau_k, v_k) & \frac{\partial F_p}{\partial v}(\tau_k, v_k) \\ \frac{\partial F_s}{\partial \tau}(\tau_k, v_k) & \frac{\partial F_s}{\partial v}(\tau_k, v_k) \end{bmatrix}^{-1} F(\tau_k, v_k) \\ &= \begin{bmatrix} \tau_k \\ v_k \end{bmatrix} - \begin{bmatrix} \frac{\partial^2 \phi_{i,j}}{\partial \tau \partial v}(\tau_k, v_k) & \frac{\partial^2 \phi_{i,j}}{\partial v^2}(\tau_k, v_k) \\ \frac{\partial^2 \phi_{i,j}}{\partial \tau^2}(\tau_k, v_k) & \frac{\partial^2 \phi_{i,j}}{\partial \tau \partial v}(\tau_k, v_k) \end{bmatrix}^{-1} F(\tau_k, v_k) \end{aligned}$$

Based on equation (7), the entries of ∇F can be easily computed as follows:

$$\frac{\partial^2 \phi_{i,j}}{\partial \tau \partial v}(\tau_k, v_k) = \begin{bmatrix} 1 & 2\tau & 3\tau^2 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 1 \\ 2v \\ 3v^2 \end{bmatrix}$$

$$\frac{\partial^2 \phi_{i,j}}{\partial v^2}(\tau_k, v_k) = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \end{bmatrix} \begin{bmatrix} a_{02} & a_{03} \\ a_{12} & a_{13} \\ a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 2 \\ 6v \end{bmatrix}$$

$$\frac{\partial^2 \phi_{i,j}}{\partial \tau^2}(\tau_k, v_k) = \begin{bmatrix} 2 & 6\tau \end{bmatrix} \begin{bmatrix} a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} 1 \\ v \\ v^2 \\ v^3 \end{bmatrix}$$

This iteration is terminated after the error $|\tau_k - \tau_{k-1}| + |\nu_k - \nu_{k-1}| + |p_k - p| + |s_k - s|$ falls below a predetermined threshold. The temperature and specific volume corresponding to the p and s values are then calculated via $T = T_i + \tau_k$ and $\nu = \nu_j + \nu_k$.

3.5 Choosing the Correct Grid Cell

For the different types of state function calculations discussed, it was assumed that all calculations are performed using the bicubic approximation coefficients associated with the correct grid cell. As the correct grid cell is not necessarily known a priori, it is essential that the correct grid cell be chosen given an arbitrary pair of thermodynamic properties such as (T, ν) , (s, ν) , or (s, p) , so that the correct coefficients $a_{k\ell}$ for the cell can be accessed. Of course, it is trivial to decide the correct cell for calculation if the given pair of states is (T, ν) , since the uniform mesh is in the $T - \nu$ domain.

For the computation that determines ν from (p, T) , the index of the correct cell is determined by following the following steps:

1. Determine i such that $T_i \leq T \leq T_{i+1}$. Let $\Delta_T = T_{i+1} - T_i$.
2. Perform a bisection search to find the index j_c such that $\frac{T-T_i}{\Delta_T} F_p(T_i, \nu_{j_c}) + \frac{T_{i+1}-T}{\Delta_T} F_p(T_{i+1}, \nu_{j_c}) - p$ is the smallest among all possible choices of j_c .
3. If $F_p(T, \nu_{j_c}) > p$, then $j = j_c - 1$. Otherwise, $j = j_c$. The index of the correct cell is $\{i, j\}$.

It is important to note that the second step is based on a linear approximation of the function F_p , and that j_c provides a good estimation on the location of the correct cell. Because $\left[\frac{dp}{d\nu}\right]_T$ is strictly negative, step 3 uniquely yields the index of the grid cell index with $F_p(T, \nu_j) \geq p > F_p(T, \nu_{j+1})$. By the continuity of F_p , it can be concluded that there exists $\nu \in [\nu_j, \nu_{j+1})$ such that $F_p(T, \nu) = p$.

Similarly, for the computation which generates T from (s, ν) , the index $\{i, j\}$ of the correct grid cell can be determined as follows:

1. Determine j such that $\nu_j \leq \nu \leq \nu_{j+1}$. Let $\Delta_\nu = \nu_{j+1} - \nu_j$.
2. Perform a bisection search to find the index i_c such that $\frac{\nu_{j+1}-\nu}{\Delta_\nu} F_s(T_{i_c}, \nu_j) + \frac{\nu-\nu_j}{\Delta_\nu} F_s(T_{i_c}, \nu_{j+1}) - p$ is the smallest among all possible choices of i_c .
3. If $F_s(T_{i_c}, \nu) > s$, then $i = i_c$. Otherwise, $i = i_c - 1$. The index of the correct cell is $\{i, j\}$.

By pre-computing and storing the values of $p(T_i, \nu_j)$ and $s(T_i, \nu_j)$, the bisection search steps can be evaluated at a relatively low computation cost. These steps can also be replaced by Newton's algorithm if low memory usage is desired.

4 RESULTS

This method for calculating refrigerant properties was implemented to evaluate its performance. The properties for superheated vapor of refrigerant R-134a were calculated over the superheated vapor region inside the rectangle $[280, 400]\text{K} \times [0.9, 10]\text{L/mol}$ in the temperature-molar volume domain over a total of 13000 test points which were selected such that these points (possibly after a conversion to the T and ν states) were uniformly distributed. The Helmholtz energy based interpolation was implemented in Matlab R2010a. The full multiparameter EOS calculation described in Tillner-Roth and Baehr (1994) and many of the algorithms described in (Lemmon *et al.*, 2010, Span, 2000) were also implemented in Matlab R2010a so that the speed of both algorithms could be accurately compared.

The computational consistency was evaluated by using the previous output of a property computation in a second computation, as described in Section 1. Three representative metrics for computational consistency are defined by

$$E_t = |T - F_T(F_s(T, v), v)|$$

$$E_v = \left| v - F_v(T, F_p(T, v)) \right|$$

$$E_{tv} = \left\| [T, v]^T - F_{TV}(F_s(T, v), F_p(T, v)) \right\|$$

The consistency errors over the examined vapor region of R-134a are illustrated in Figures 2-4. These results are quite good, as the errors are all below 10^{-12} .

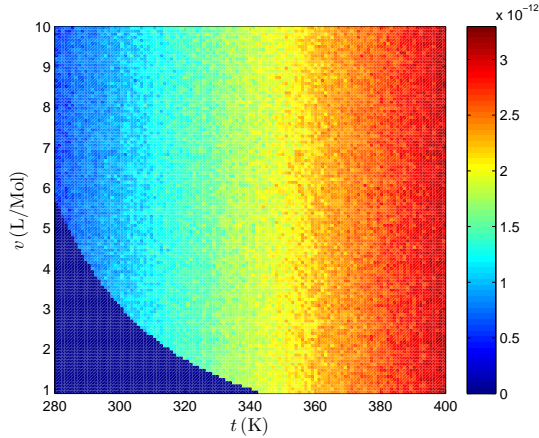


Figure 2: Computation consistency error: E_t .

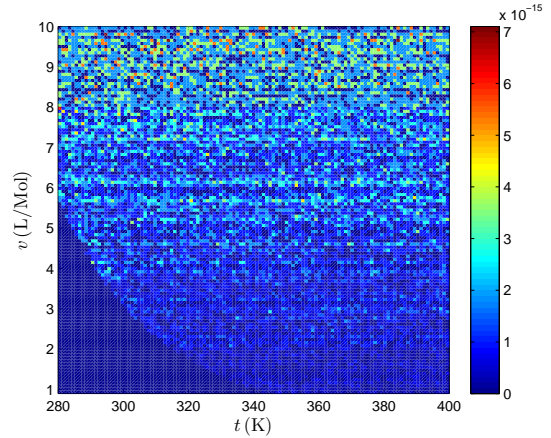


Figure 3: Computation consistency error: E_v .

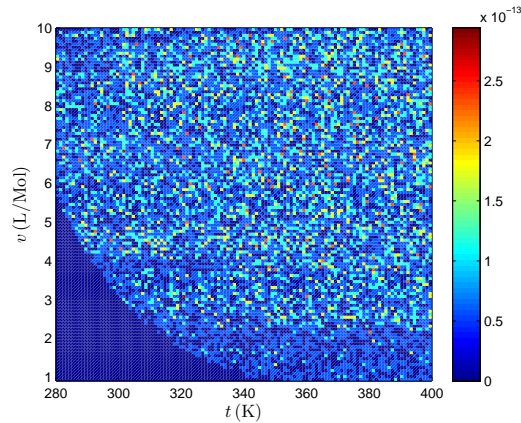


Figure 4: Computation consistency error: E_{tv} .

Table 1 shows the computation speed of the new method, as well as the impact of base mesh size on the computation speed. Three different size meshes were used: Mesh 1 was 50 points by 100 points, Mesh 2 was 100 points by 200 points, and Mesh 3 was 200 points by 400 points. As expected, the first class of calculations, described in Section 3.2, are the most efficient since they only require the evaluation of very low order polynomials, and the grid cell allocation requires very little computation. The second class of calculations, described in Section 3.3, performs analytic root computation for quadratic functions, and are about 4-40 times slower than the first class. For this class of calculations, grid cell allocation requires a considerable amount of computation when the mesh size is large. The third class of calculations, described in Section 3.4, is the least computationally efficient due to the iterative nature of Newton's method.

		Average computation time (ms)		
		Mesh 1	Mesh 2	Mesh 3
Type 1	$(T, v) \rightarrow s$	7.56E-03	7.37E-04	7.50E-04
	$(T, v) \rightarrow p$	7.43E-03	7.43E-04	8.61E-04
Type 2	$(s, v) \rightarrow T$	2.99E-02	3.09E-02	3.25E-02
	$(T, p) \rightarrow v$	2.95E-02	3.08E-02	3.48E-02
Type 3	$(s, p) \rightarrow (T, v)$	0.364	0.546	1.24

Table 1: Computation time for different mesh sizes.

Table 2 compares the speed of the standard Newton-based method to the Helmholtz energy interpolation-based method in terms of the calculation of ρ from (T, p) . The baseline for comparison is computed using the EOS method where the convergence criterion is that $|\rho_n - \rho_{n-1}| < 1E-12$. The interpolation-based methods are computed using the same meshes as in Table 1, while the Newton-based EOS results are computed for the same test points with different tolerance settings (1E-8, 1E-5, 1E-3). e_r is the relative error as compared to the baseline data. On average, the interpolation-based method is about 53 times faster than the Newton-based EOS method.

Newton-based EOS method		Interpolation-based method	
Time (ms)	e_r	Time (ms)	e_r
1.92	9.91E-09	2.95E-02	2.98E-4
1.70	9.98E-06	3.08E-02	1.84E-5
1.42	9.85E-04	3.48E-02	6.28E-6

Table 2: $(T, p) \rightarrow \rho$ calculation relative error comparison.

5 CONCLUSIONS AND FUTURE WORK

This paper described a new method for calculating a range of thermodynamic properties of refrigerants which used the interpolation functions to describe the surface of the Helmholtz energy A . This method has three particularly useful characteristics; it is much faster than standard Newton-based EOS methods, it is quite accurate, and the property calculations are consistent.

This work could potentially be extended in a variety of directions. While the computations performed in this paper were limited to the superheated vapor region for the sake of simplicity and verification of the underlying premise upon which this method was based, it would be quite useful to extend these computations to other regions of the phase plane, such as the subcooled liquid region, the supercritical region, and the two-phase region. It would also be very useful to explore the creation of interpolation functions for other fundamental equations of state, such as the Gibbs energy. One of the principal limitations of the method, as discussed in this paper, is that Newton iterations are required for some combinations of independent variables (such as calculating (T, v) from (s, p)). Other fundamental equations of state could be much faster when using (s, p) as independent variables; just as the base independent variables for A are temperature and density, other fundamental EOS have different independent variables. It could thus be quite productive to identify the optimal fundamental EOS for a particular application.

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